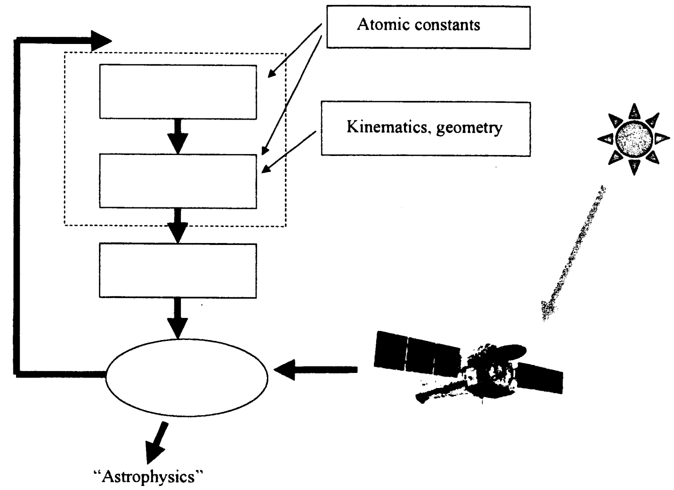
Atomic Calculations and Laboratory Measurements Relevant to X-ray Warm Absorbers

Tim Kallman (NASA/GSFC)

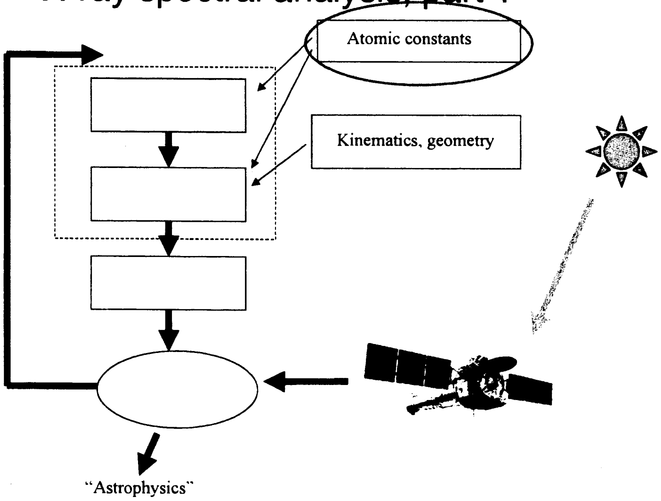
+

M. Bautista & C. Mendoza (IVIC, Venezuela,
P. Palmeri (Mons, Belgium)

X-ray spectral analysis, part 1



X-ray spectral analysis, part 1



How did we get here?

1996: rates, codes and astrophysics
1999: atomic data needs for X-ray Astronomy
2005: XDAP

then: raymond-smith: 49.8 kbytes
now: atomdb: 135 Mbytes

theoretical tools

Packages:

- Cowan/ HFR
- Z expansion
- MCHF
- MCDF/GRASP
- Hullac
- fac
- Autostructure/superstructure
- Rmatrix

Features:

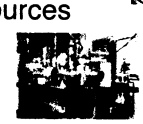
- Configuration interaction/superposition of configurations
- Non-orthogonal orbitals
- Semi-empirical corrections
- Fully relativistic or Breit-pauli approximation to relativistic hamiltonian
- Coupled to collisional-radiative code; very efficient caculation of radial part of matrix elements
- Distorted wave scattering
- Scattering: continuum wavefunctions calculated in close-coupling approximation

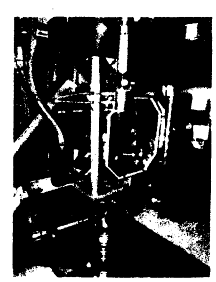
The algorithms are not new, but are enabled on a large scale by computing improvements

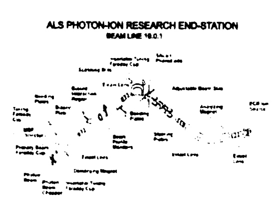
+ Databases: Chianti, atomdb, ornl, adas, topbase

Experimental tools

- Traps (ebit)
- Storage rings
- Synchrotron light sources
  - (+beams)

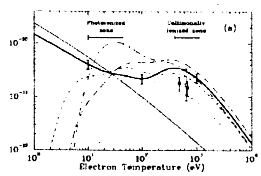






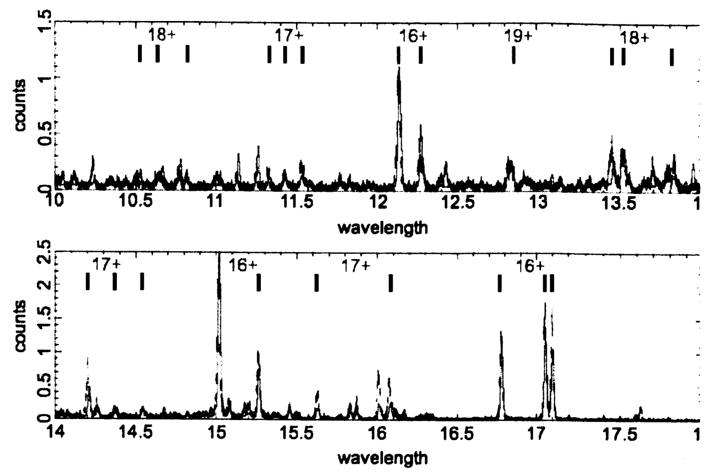
Dielectronic recombination

- challenges:
  - DR is a resonant process, need accurate resonant energies
- Storage ring and ebit measurements: all L-shell ions of iron, M-shell under way (Savin et al.; Muller; Schippers ...
  - These are key for verifying theory, and for demonstrating the importance of accurate resonance structure
- Calculations:
  - Fac: total DR rates for H-Ne isosequences
  - Autostructure: state-resolved rates for isosequences He-Na (?)-like ions for elements He-Zn. (Badnell, Zatsarinny, Altun et al...)
  - Agreement with each other, and experiment, is ~20%

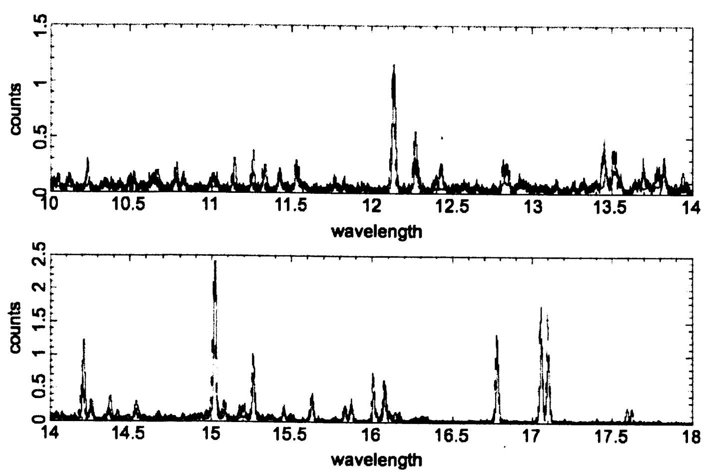


Fe 18+-Fe17+ Savin et al. 2002

Sample fit to HETG Capella spectrum; xstar ionization balance

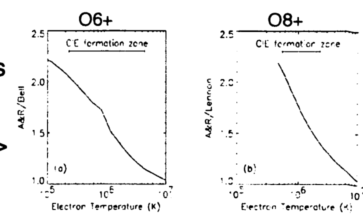


Sample fit to HETG Capella spectrum; DR perturbed by 30%

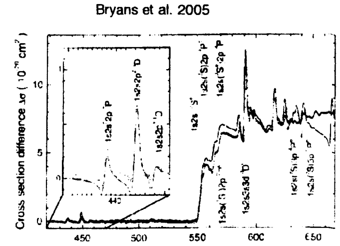


Collisional ionization

- Challenges:
  - Rate from ground state is all that is needed for many purposes--> experiments can be used directly
  - Lotz --> Arnaud and Rothenflug --> Arnaud and Raymond --> Mazzotta: fit to early measurements... discrepancies?
  - Metastables can dominate
- Storage ring experiments (Muller et al.)
  - Can eliminate metastables, due to 'cold' beam
  - Reveal important effects: REDA, EA



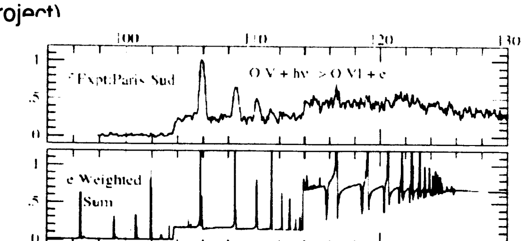
Bryans et al. 2005



O5+; Muller et al. (2000)

Photoionization cross sections

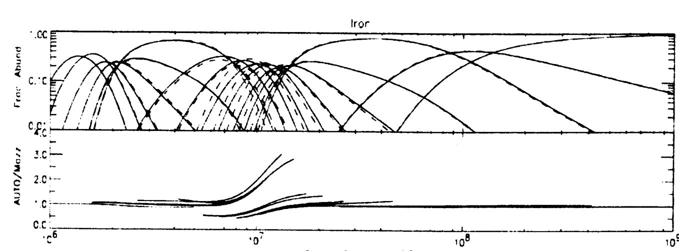
- Challenges
  - Need for inner shells, excited states (<--> RR)
  - Importance of resonances
- Experiment:
  - Synchrotron/ion beams
- calculations
  - Rmatrix (iron project)
  - autostructure



Champeaux et al. 2003; Nahar 2004

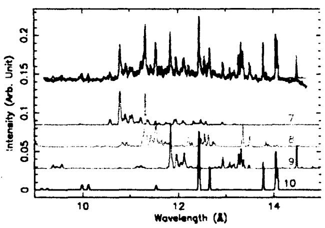
Ionization balance

- Bryans et al. 2005
  - Put together Autostructure DR rates+ collisional ionization rates for elements

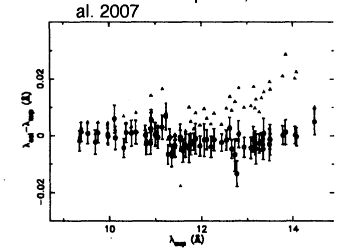


spectra

- Accurate wavelengths are key to line ids, and to anchoring semi-empirical structure calculations
- Theoretical calculations are not (generally) accurate enough to distinguish lines in rich X-ray spectra
- Lab measurements are key
  - Ebit has been a leader in this field



Ni L-shell ion spectra; Gu et al. 2007

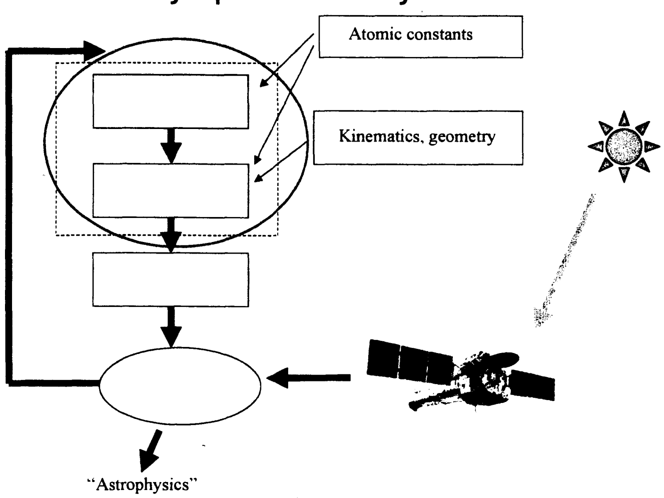


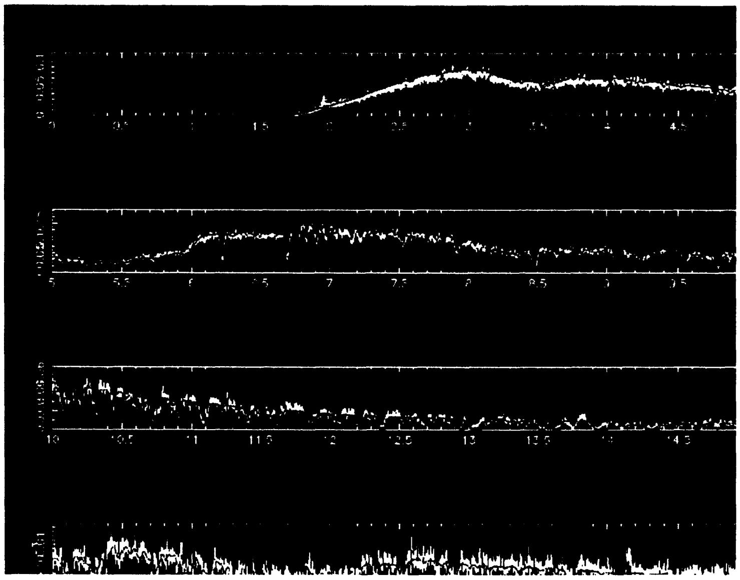
Calculated vs. measured line wavelengths

Needs

- Auger
  - Following inner shell ionization, cascade of electrons
  - Correlated line emission?
- Charge exchange: ‘non-traditional’ X-ray sources: planets, solar system objects
- Trace elements
- Protons
  - Thermal: angular momentum changing collisions
  - Non-thermal: spectral signatures of cosmic rays.
- Dust/molecules/low ionization gas: inner shells
- Inner shells: inner shell lines, photoionization cross sections, collision strengths
- Collisional ionization: loose ends?
- Collisional processes away from equilibrium peak?

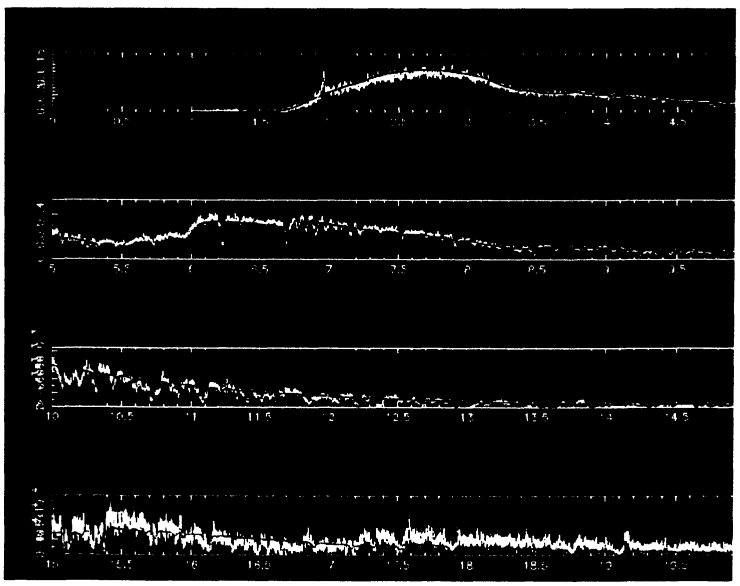
X-ray spectral analysis

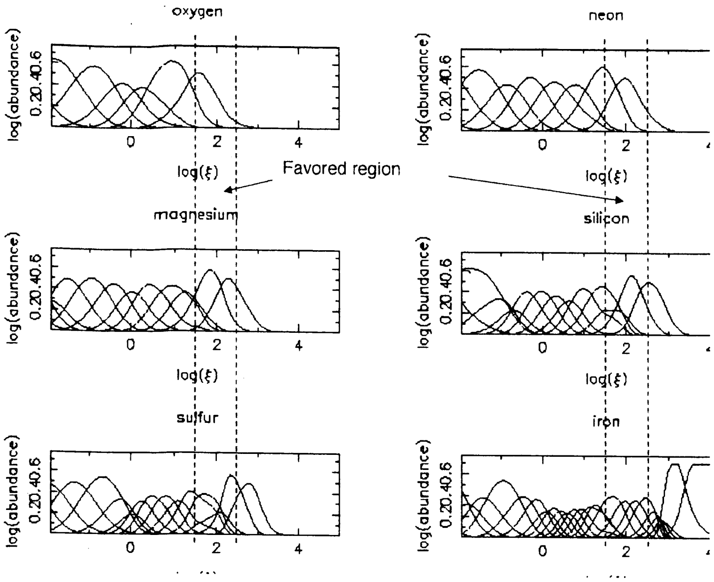




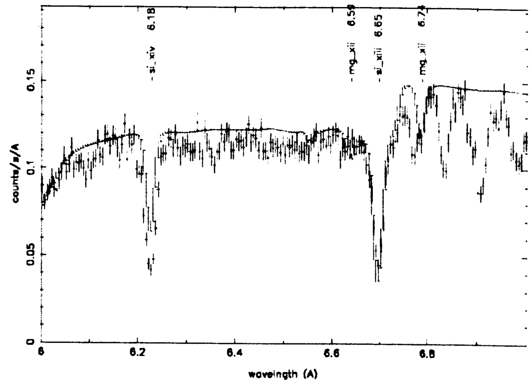
photoionized models

- Start with a single photoionized component
- pure absorption
- Choose single turbulent width to fit majority of lines,
- v_{turb}=300 km/s
- use z=0.007, compare with $z_{ngc3783}$=0.00938
- --> $v_{outflow}$=700 km/s
- Best fit ionization parameter: $\log\xi\sim2$.

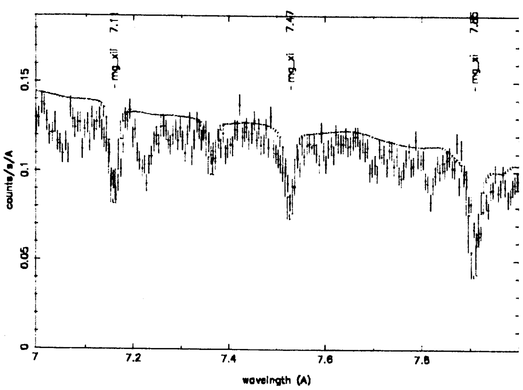




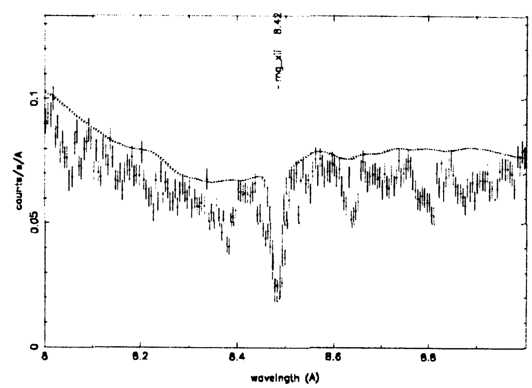
Si VII-XI K lines

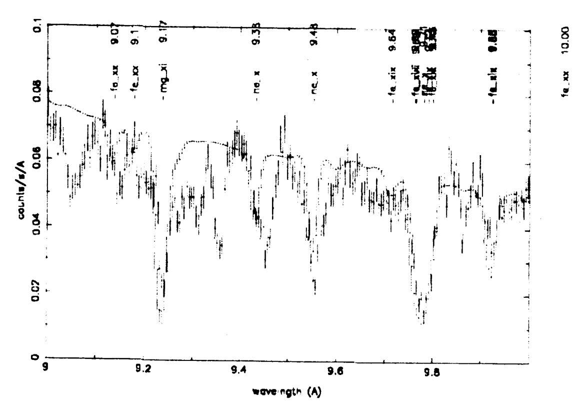


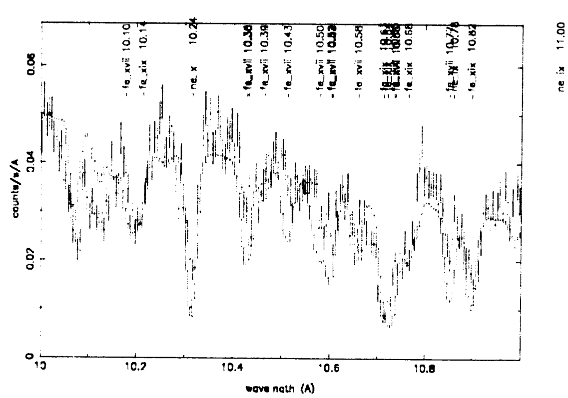
Al XIII Al XII



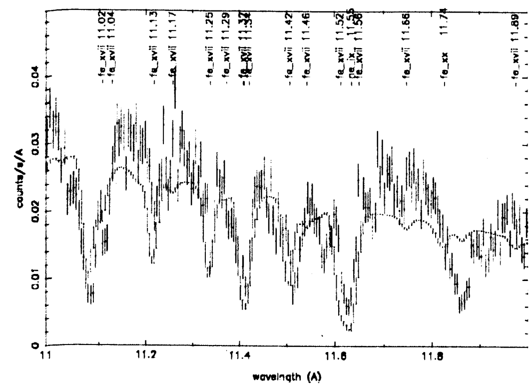
Fe XX-XXII



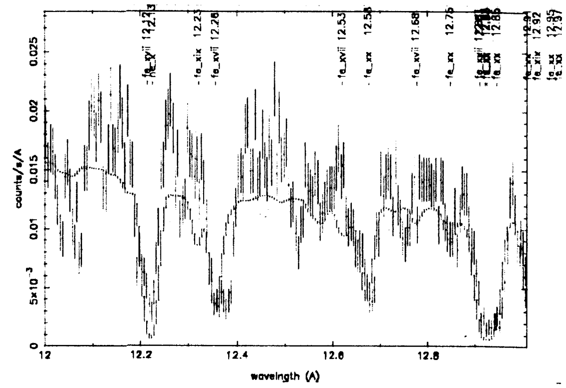


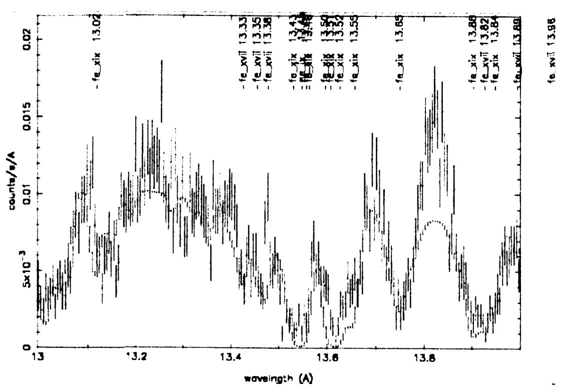


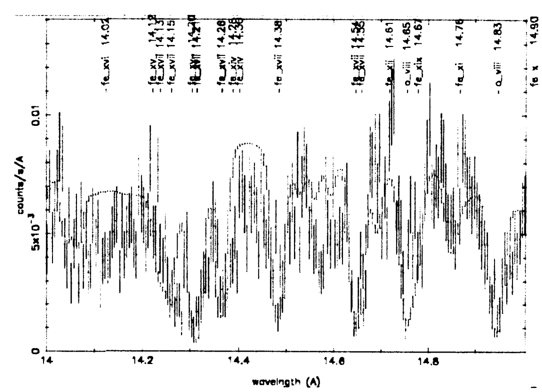
Fe XXII



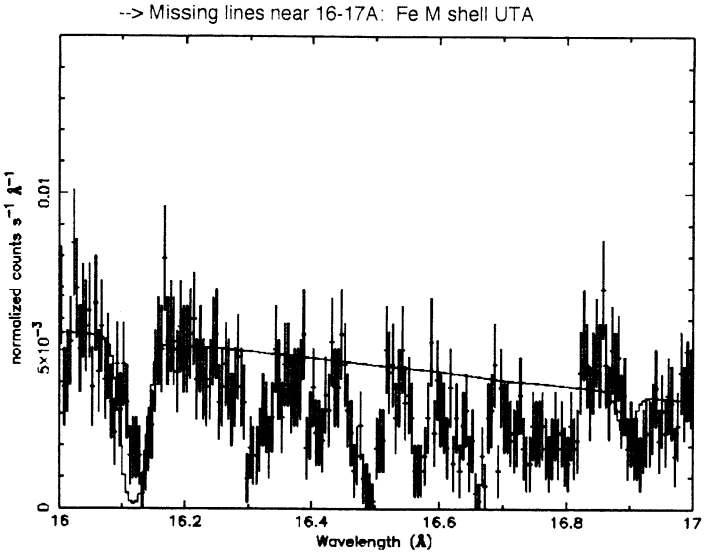
Fe XXI





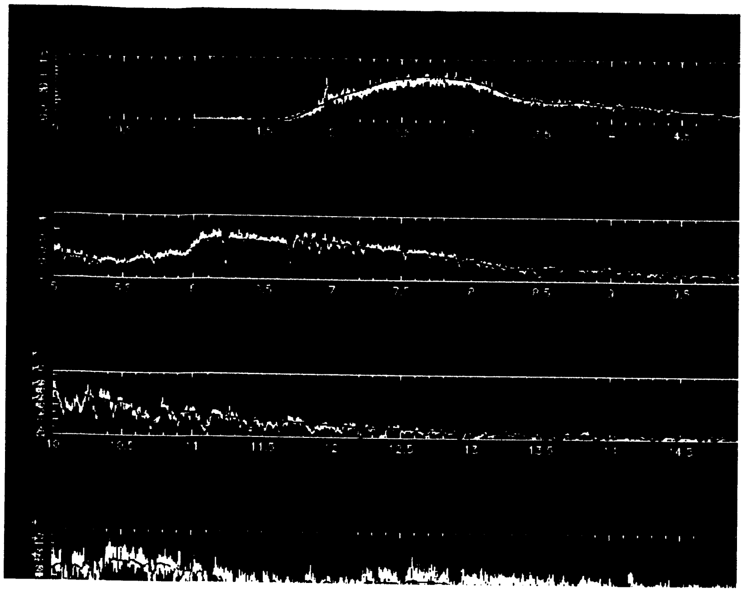


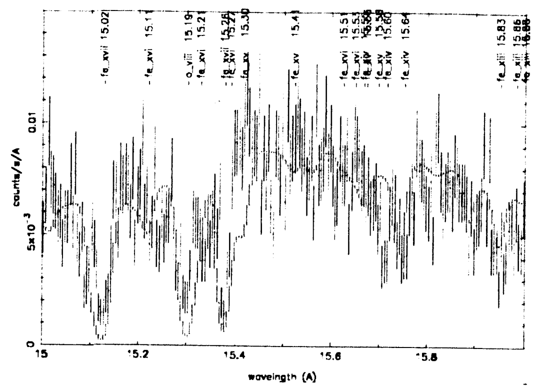
--> Missing lines near 16-17A: Fe M shell UTA

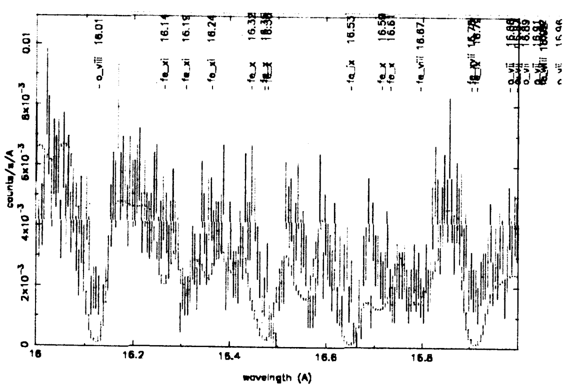


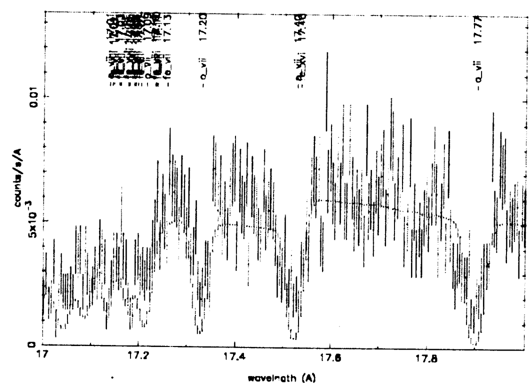
pure absorption photoionized models: multiple ξ components

- 2 Component Fit,
  - logξ~2. (as before)
  - logξ~ 0. (produces Fe M shell UTA)
- Other parameters the same as single component:
  - z=0.007,
  - v_{turb}=300 km/s

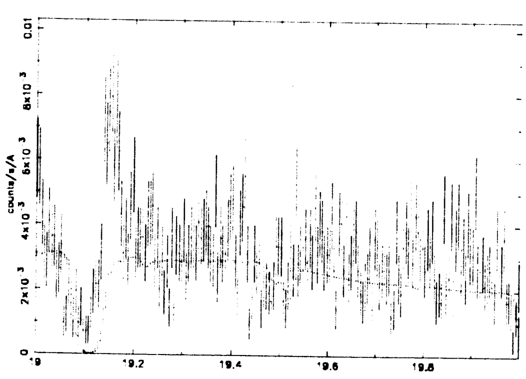


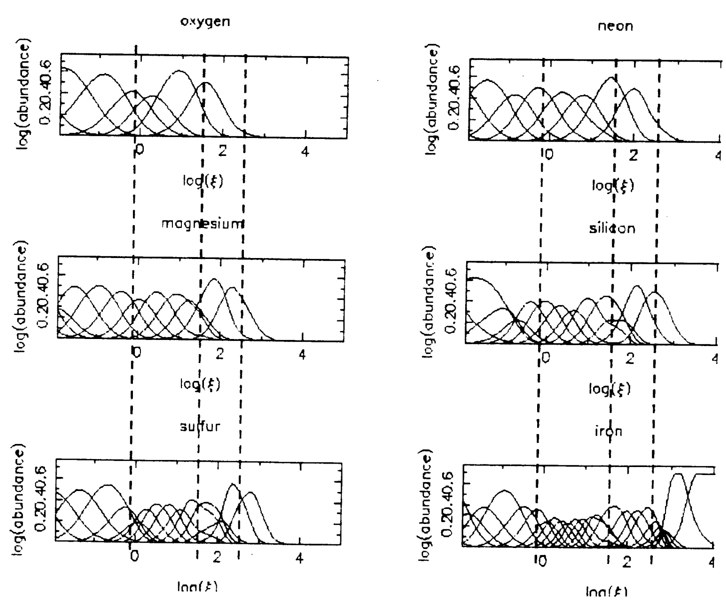




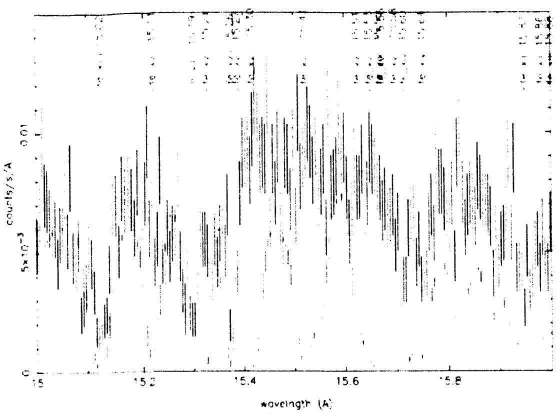


O VIII Lα: emission component





What if we try a Continuous distribution of ionization parameter, 0.1<logξ<2.4?



--> Complete ruled out

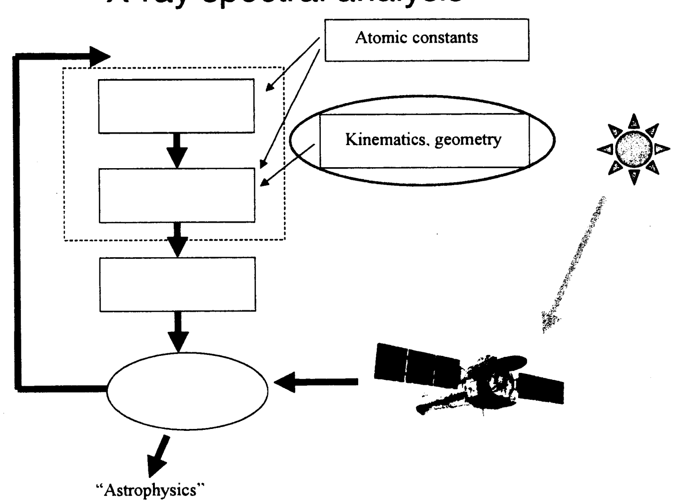
'Photoionization Models'

- Full global model
- (i.e. photoionization-->synthetic spectrum --> xspec --> fit)
- Xstar version 2.1ln2
  - Inner M shell 2-3 UTAs (FAC; Gu); >400 lines explicitly calculated
  - Chianti v. 5 data for iron L
  - Iron K shell data from R-matrix calculations(Bautista, Palmeri, Mendoza et al)
  - Available from xstar website, as are ready-made tables
- Not in current release version, 2.1kn7
- Other models have similar ingredients
- Xspec 'analytic model' warmabs
  - Not fully self consistent: assumes uniform ionization absorber, but this is small error for low columns.
  - http://heasarc.gsfc.nasa.gov/xstar/xstar.html

Comparison of photoionization models

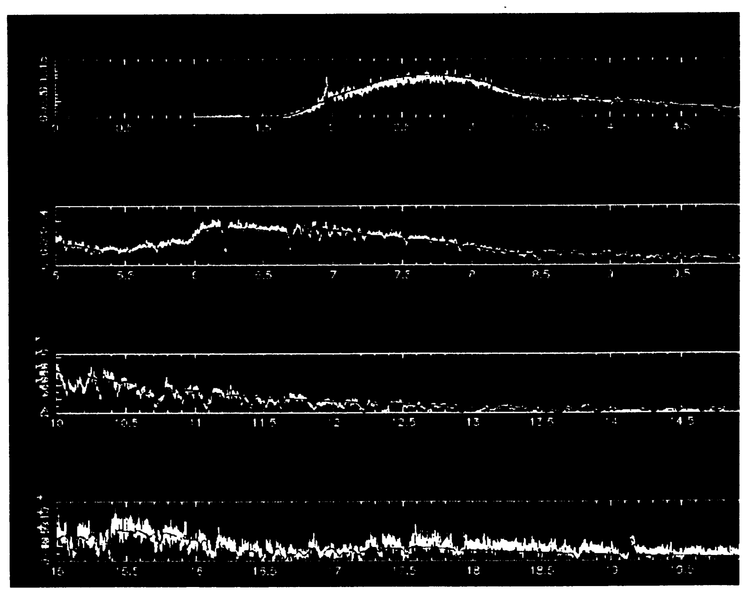
	X*release (2.1kn4)	X* beta (2.1ln2)	warmabs	Warmabs 2.1ln2	Other: phase	Other: titan	photoion
Xspec interface	talbles	tables	analytic	analytic	?	?	analytic
Atomic data	KB01	KB01, K04, chianti	KB01	KB01, K04, chianti	apec	?	Hullac/fac
'real slab	y	y	n	n	?	y	n
Self consistent SED	y	y	n	y	?	y	n
nlte	y	y	y	y	?	y	y
Radiative transfer	n	n	n	n	?	y	n
'dynamics'	n	n	n	(y)	?	?	n

X-ray spectral analysis



Now try absorption + thermal emission photoionized models

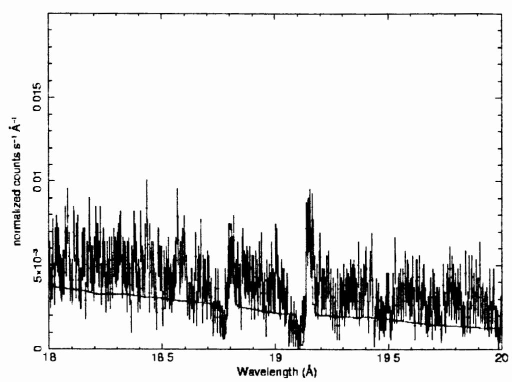
- Add component due to 'thermal' photoionization (i.e. Recombination+collisional excitation processes): 'photemis'
- Component has redshift z=0.009, I.e. redshift of object



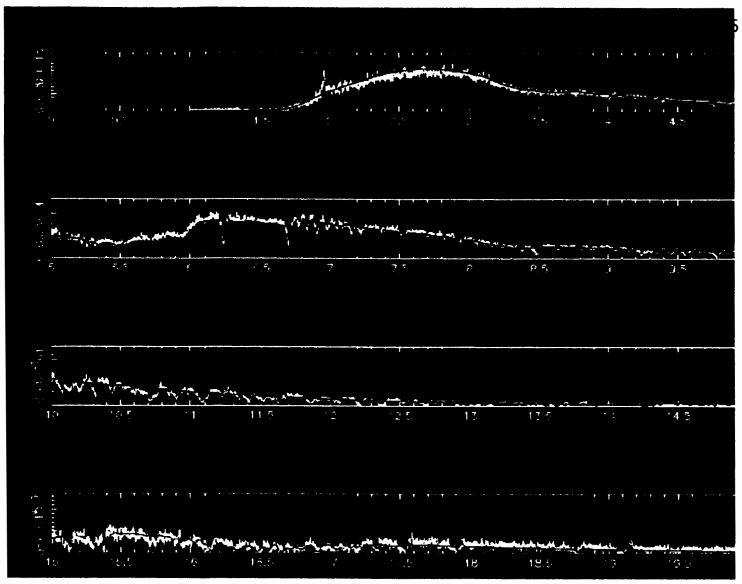
Now try photoionized scattering models

- Photemis model does not account for scattered emission
- To test this, we apply method from theory of hot star winds, (SEI) method (Lamers et al. 1992) assumes ordered, radial supersonic flow
- Apply SEI profile to all spectrum lines, with depth parameter proportional to depth calculated by warmabs.
- Free parameter is ratio of scattered emission to absorption, C.

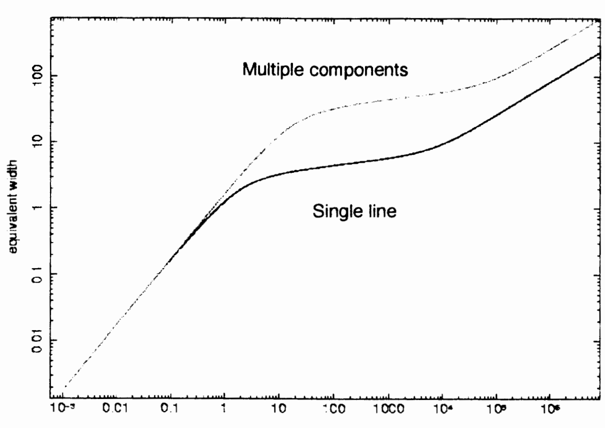
Wind models



O VIII Lα requires C~1



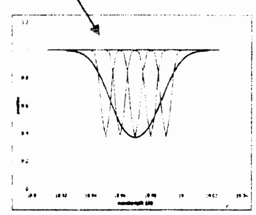
This affects the Curve of growth; eg. For O VIII Lα, v_{turb}=300, v_{therm}=60, C=1, a=0.01

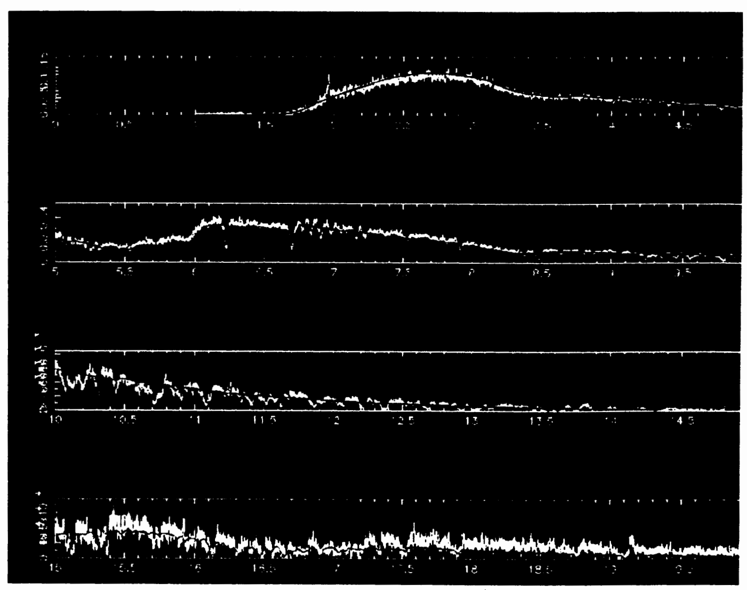


Now try multicomponent models

- UV spectra show some X-ray warm absorber lines correspond to multiple narrow components in the UV
- Multabs is an attempt to test whether multiple discrete components can mimic a single feature.
- Several identical warmabs components, each with thermal width are spread evenly across an energy interval determined by vturb
- The number is determined by a 'covering fraction', C=1 corresponds to a black trough, C=0 corresponds to one thermal component

$N_{components}=C\, v_{turb}/v_{therm}$



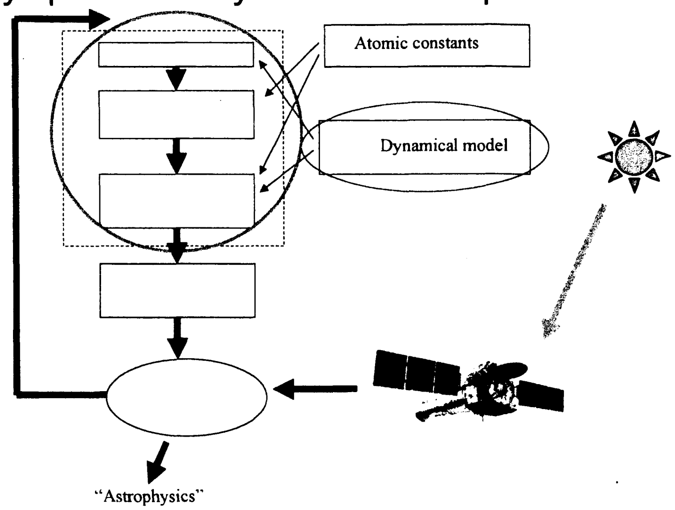


A summary of χ^2/8192

Gaussian notch	11945
Single component absorption	16093
2 component absorption	15186
+photemis	15161
Wind, C=1	21626
multabs	18974

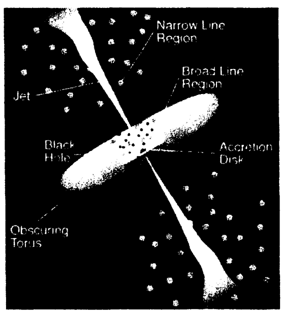
The pure absorption 2 component model looks best...

X-ray spectral analysis: a different procedure



dynamical models: torus winds

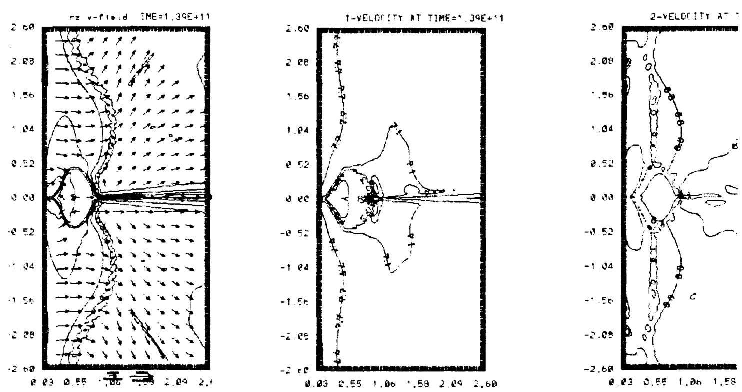
- Following suggestions by Balsara and Krolik (1984), Krolik and Kriss (1996)
- Assume a torus at 0.1 pc about a $10^6 M_{sun}$ black hole
- Initial structure is constant angular momentum adiabatic (cf. Papaloizou and Pringle 1984)
- This structure is stable (numerically) for >20 rotation periods
- Choose $T<10^4$K, $n\sim10^8$ cm^{-3} for unperturbed torus
- Calculate dynamics in 2.5d (2d + axisymmetry) using zeus-2d



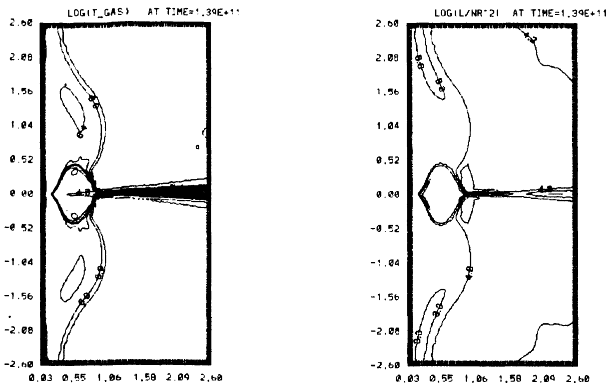
dynamical models: torus winds

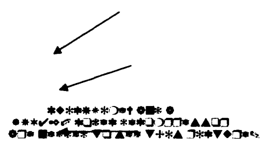
- Add illumination by point source of X-rays at the center
- Include physics of X-ray heating, radiative cooling --> evaporative flow (cf. Blondin 1994)
- Also radiative driving due to UV lines (cf. Castor et al. 1976; Stevens & K. 1986)
- Formulation similar to Proga et al. 2000, Proga & K. 2002, 2004

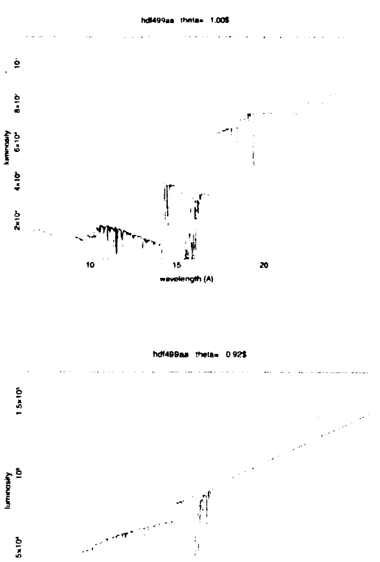
Velocity and density fields

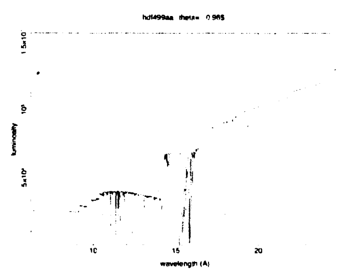


Temperature and ionization parameter









Sample spectra look ~like warm absorbers

results

- Find strong evaporative flow, $\dot{M}$~10^{-5} M_{sun}/yr
- Initial flow is inward from illuminated face
- Later flow is isotropically outward as torus shape changes
- T_{comp}~10 T_{esc}; t_{heat} << t_{rot}
- Find gas at intermediate ionization parameters
- Match to data? Region of warm flow is narrow

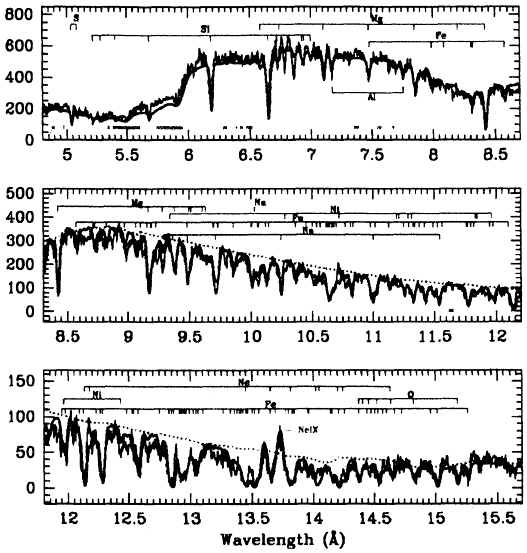
Extra slides

Comparison with previous work

	Netzer	Krongold	Blustin	Me
Log(U)	-0.6,-1.2	0.76		0.45
Log(ξ_1)	3.7,3.1	2.25	2.4	2.2
Log(N_1)	22.2	22.2	22.45	21.4
Log(U)	-2.4	-0.78		-1.55
Log(ξ_2)	0.69	0.72	0.3	0.2
Log(N_2)	21.9	21.6	20.73	20.4

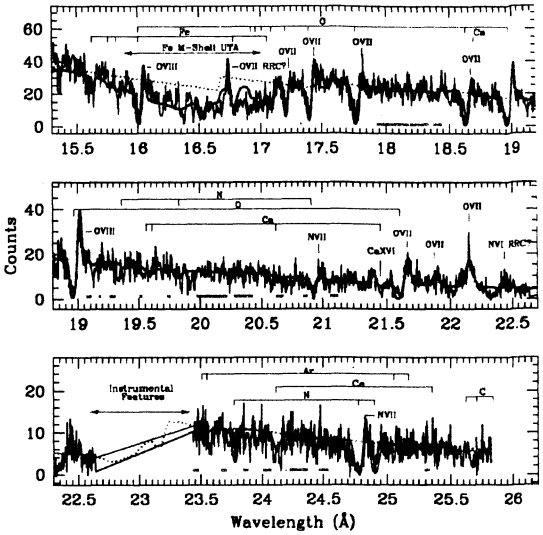
Krongold et al 2004

.>100 absorption features
.blueshifted, v~800 km/s
.broadened, .vturb~300 km/s
.emission in some components
.fit to 2 photoionization model components
.Fe M shell UTA fitted using Gaussian approximation
.Full global model



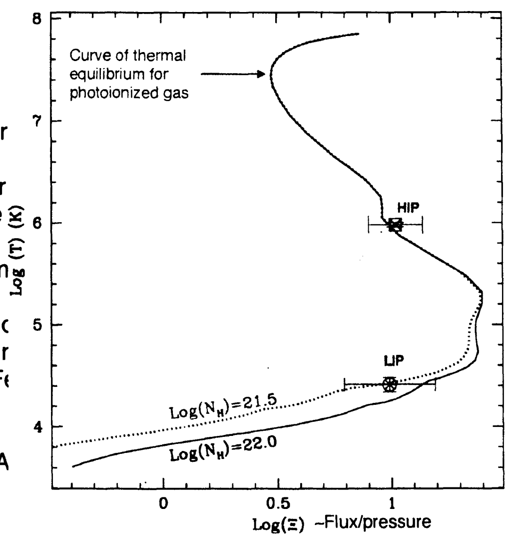
Krongold et al 2004

.>100 absorption features
.blueshifted, v~800 km/s
.broadened, .vturb~300 km/s
.emission in some components
.fit to 2 photoionization model components
.Fe M shell UTA fitted using Gaussian approximation
.Full global model



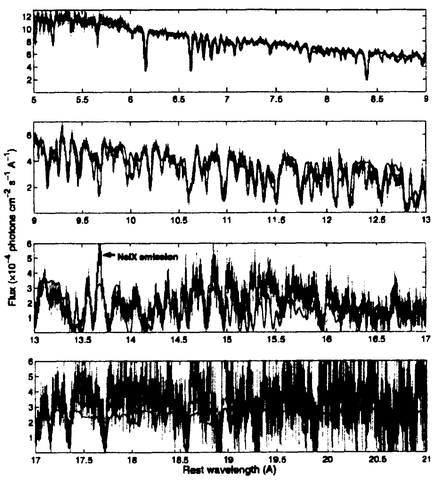
Krongold et al 2004

.fit to 2 photoionizatior model components
.Ionization parameter and temperature are consistent with coexistence in the sam physical region
.Disfavored existence c intermediate ionizatior gas due to shape of Fe M shell UTA
.But used simplified atomic model for UTA



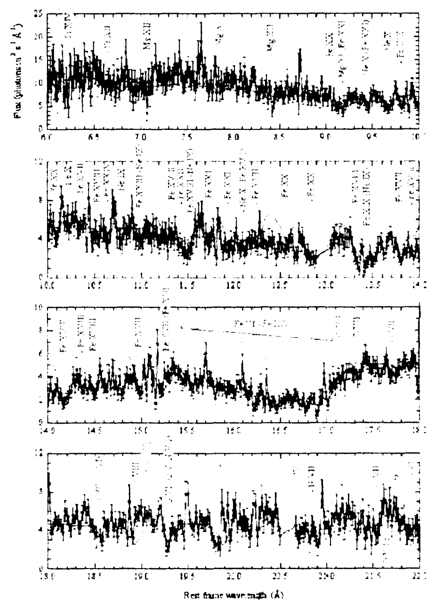
Chelouche and Netzer 2005

_Combined model for dynamics and spectrum
_Assumes ballistic trajectories
_Favors clumped wind



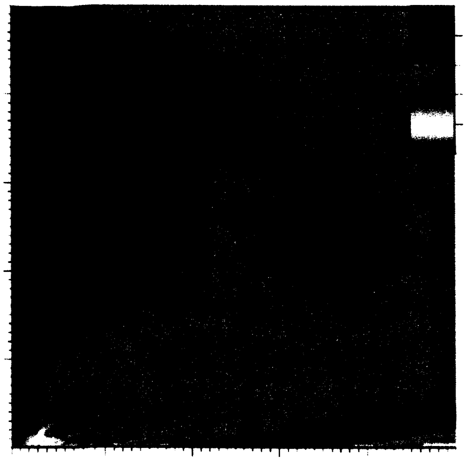
Blustin et al. (2004)

.Fitted the XMM RGS spectrum using global model
.Also find evidence for two components
.Omit Ca
.Include line-by-line treatment of M shell UTA, but still miss some
.Claim evidence for higher ionization parameter material
.require large overabundance of iron



- Work so far on fitting warm absorber spectra has concentrated on the assumption of a small number of discrete components
- This places important constraints on the flow dynamics, if it is true
- There is no obvious a priori reason why outflows should favor a small number or range of physical conditions
- In this talk I will test models in which the ionization distribution is continuous rather than discrete, and discuss something about what it means
- Previous tests of this have invoked simplified models for the Fe M shell UTA which may affect the result

ids have smooth density distributions on the scales which can be
ed...



Proga and Kallman 2004

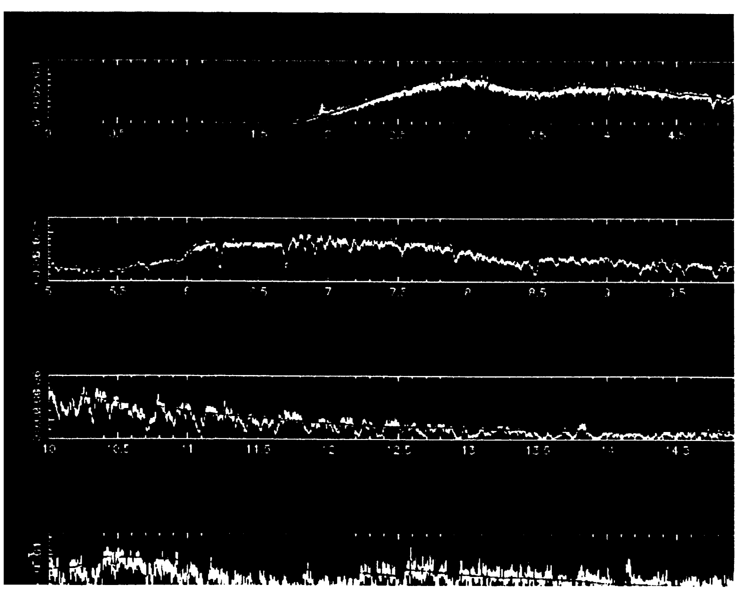
Comparison of model properties

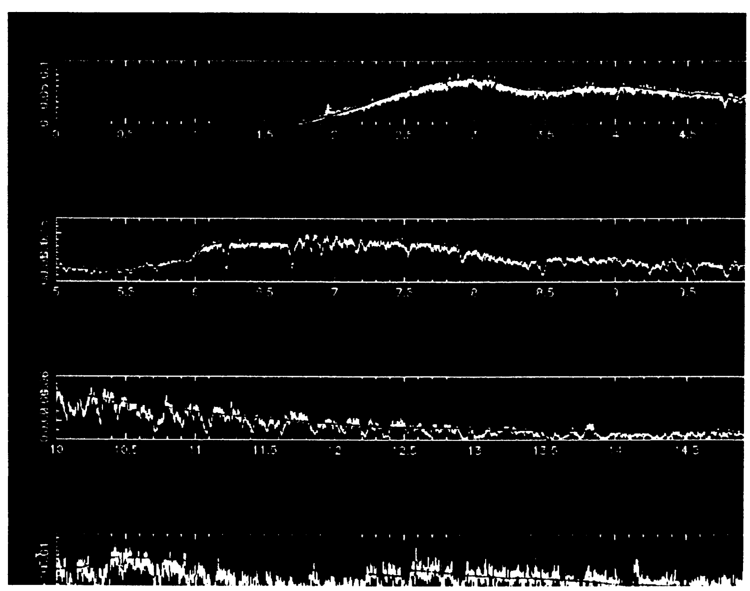
	X* release (2.1kn4)	X* beta (2.1l)	warmabs	Others (titan apec)
Xspec interface	tables	tables	analytic	various
Atomic data	KB01	KB01, K04, chianti5	KB01,K04, chianti5	various
'real' slab	y	y	n	various
Energy resolved	?	?	y	various
Self-consistent SED	y	y	(y)	(y)
nlte	y	y	y	y
radiative transfer	n	n	n	y
dynamics	n	n	(y)	n

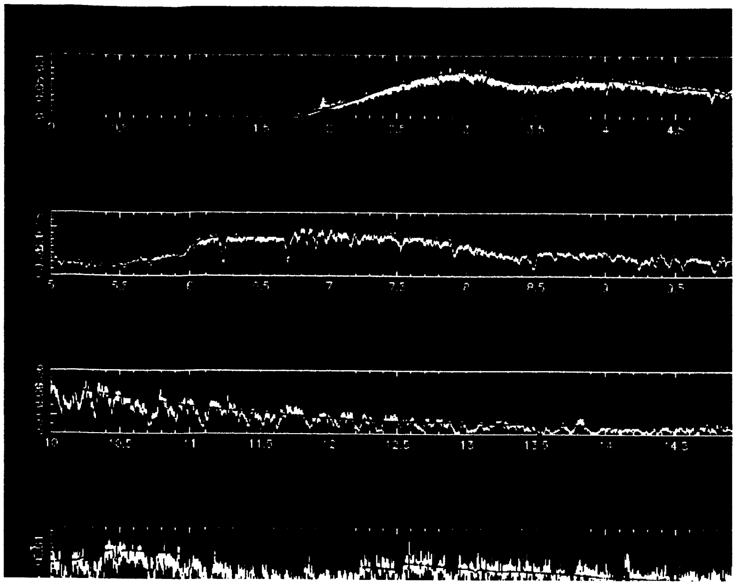
- Examples of (2)
  - How well do we do? Warm absorber example
  - What's wrong?
    - Atomic data incompleteness
    - Atomic data errors
    - Incorrect physical assumptions
- Some areas of recent progress
  - Combined emission/absorption models
  - Thermal emission
  - Scattered emission
- Things to watch out for
  - Finite resolution
  - Granularity
  - emission/absorption tradeoffs
- Some areas of recent progress

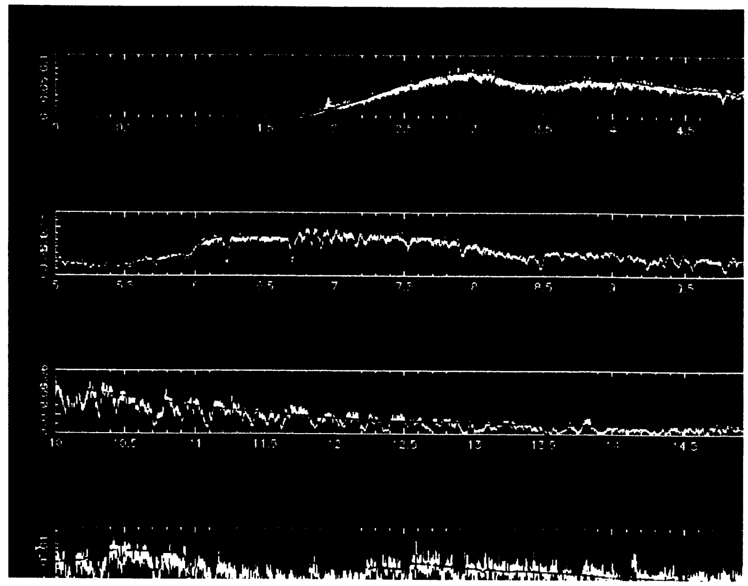
1) simple models: gaussian notches

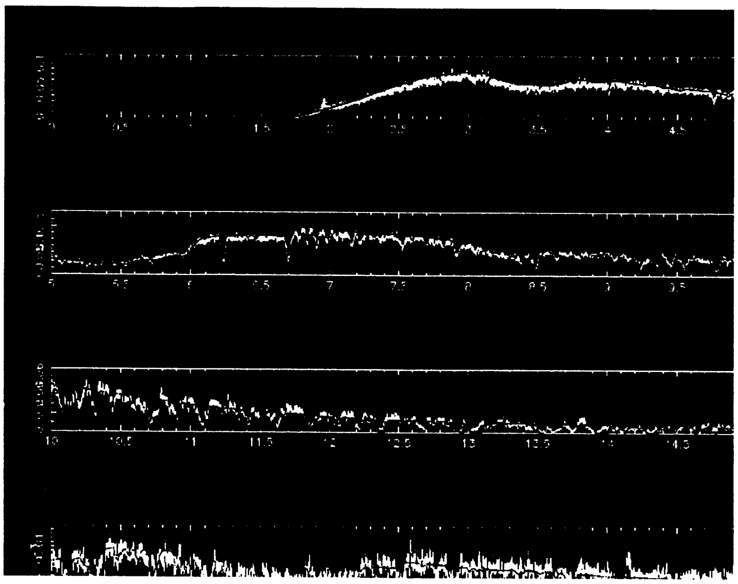
- As a start, fit to a continuum plus Gaussian absorption lines. Choose a continuum consisting of a power law +0.1 keV blackbody + cold absorption
- Absorption lines are placed randomly and strength and width adjusted to improve the fit.

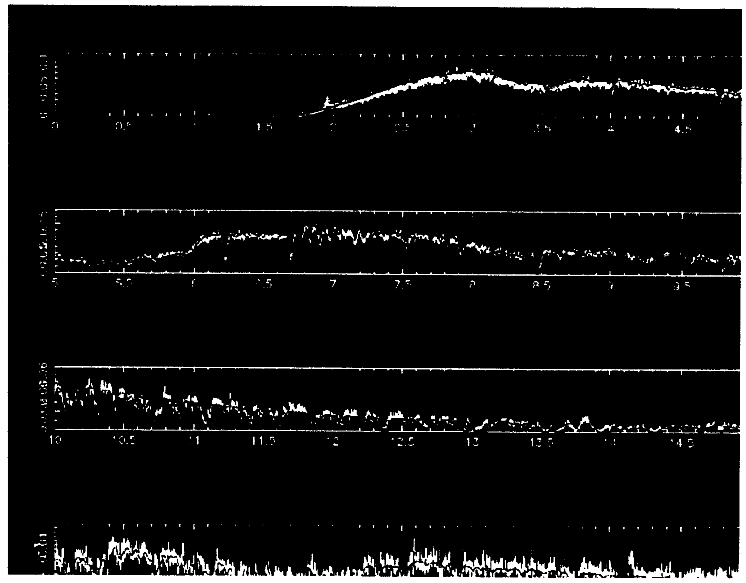






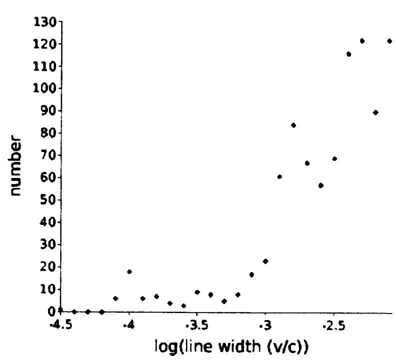




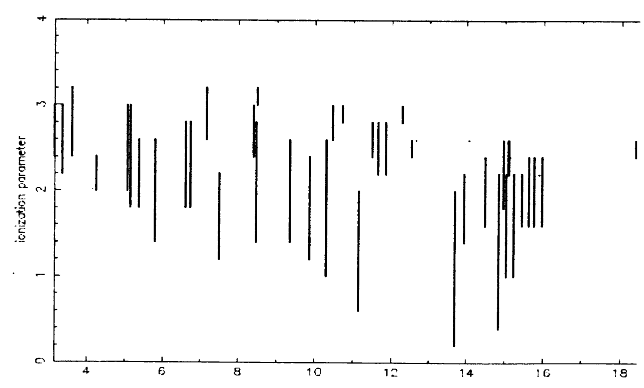


Results of notch model:

- requires ~950 lines
- Ids for ~100
- 300 km/s<v/c<2000
- Allows line Ids
- Shows distribution of line widths, offsets



Ionization parameter of maximum ion abundance vs. line wavelength for identified lines



--> statistics of the line widths implies bound on velocity, v<1000 km/s: small number of components of photoionized gas